Swami Ramanand Teerth Marathwada University, Nanded

"Solution Thermodynamics of Adenine, Thymine and Their Sugar Derivatives in Different Aqueous Media"

In the Subject

Chemistry Faculty of Science & Technology

Submitted by

Mr. Rohidas Vyankatrao Dudhate

(M. Sc., Chemistry)

Under The Supervision of

Dr. Santosh D. Deosarkar

(M. Sc., Ph.D., SET)

Professor

School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded

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2. Title of the research problem.

"Solution Thermodynamics of Adenine, Thymine and Their Sugar Derivatives in Different Aqueous Media"

3. Name of the Research Scholar with detailed address for correspondence, contact number, email-id, etc

Name of Research Scholar	Address	Email-id	Contact Number
Rohidas Vyankatrao Dudhate	School of Chemical Sciences, S. R. T. M. University, Nanded-43143 606 (MS) India	dudhaterohi@gmail.com	7507747483

4. Name of the Research Supervisor, Co-Supervisor (if any), Research Centre, detailed address for correspondence, contact number, email-id, etc.

Name of Research Supervisor	**Research Centre**	Email-id	Contact Number
Prof. Dr. Santosh D. Deosarkar	School of Chemical Sciences, S. R. T. M. University, Nanded-43143 606 (MS) India	sandeo24@srtmun.ac.in	9096403856

5. Introduction to the proposed work

The thermodynamic properties of nucleic acid bases (NABs) and nucleic acid bases (NABSDs) in different aqueous media are crucial for understanding their behavior in biological systems, particularly in the context of nucleic acids like DNA and RNA. These molecules, which are components of the genetic code, interact with water and other solutes in biological environments. Nucleic acids are differ from proteins in the sense of chemical component due to the hydrogen (–H) bond are key to secondary structure formation are between the variable moieties rather than backbone. The backbone of nucleic acids is more flexible than proteins. Determination of nucleic acid-proteins, nucleic acid-drugs, nucleic acid-salt and nucleic-solvent interactions are important in the varieties of filed such as

nucleic acid/protein chemistry, medicine, genetics, biotechnology and structure and stability studies of DNA/RNA. Nitrogenous base and their Nucleosides is the monomer unit of RNA/DNA and are involved in several biochemical processes such as cell bioenergetics, cellular metabolism, cancer marker, diagnostic marker of HIV and signal transduction pathways. It is used to mimic behavior of nucleic acids in living organisms.

Thermodynamic properties of solution containing NABs and NABSDs in different aqueous media provide the significant information to infer the understanding associations and complexiation behavior, related structural changes and complex formation, conformational changes and denaturation in biochemical reactions within living organisms. The measurement of densities, ultrasonic velocities, refractive indices and viscosities provide very useful techniques for gaining qualitative information about the solutions properties. Studies on interactions of polar, non-polar compound in solution are significant and important tool for pharmaceutical industries, proteins/vitamins chemistry, technical process, denaturation/renaturation structure of DNA/RNA and complex physiological processes in living cell such as immune function, oxygen transport and muscle contraction becomes the base of these interactions. It is interesting to observe the interactions between NABs/NABSDs in water and different aqueous media containing selected cosolutes such as amino acids, vitamins, electrolytes and non-electrolytes, drugs etc.

One approach that may help in understanding about the nature of nucleic acid-proteins, nucleic acid-drugs, nucleic acid-salt, nucleic-vitamins and nucleic acid-solvent interactions through volumetric, acoustic and viscometric properties. A variety of chemical substance cause changes in conformational changes and denaturation/renaturation structure of DNA/RNA when present in nucleic acid-solvent solution. The complex conformation and factors affecting the structure of DNA/RNA in solution make the direct study of nucleic acid interactions is difficult. Therefore, one less complex measurements technique is to study of aqueous solution of NABs/NABSDs interaction with vitamins, sugar, salt and useful pharmaceutically active drugs in aqueous solution provide very important information of solute-solvent/solute interaction and hydration behaviour of NABs/NABSDs that are significant in understanding the stability of nucleic acid.

6. Review / survey / present status of the work carried out in the field at National and International level

The thermodynamic properties and molecular interactions in aqueous solutions of nucleic acid bases and their sugar derivatives (nucleosides and nucleotides) are extensively studies

by number of researchers. In view of the chemical and biological significance of these compounds, they have been studied in aqueous solutions of different co-solutes and co-solvents through volumetric, acoustical, and transfer properties and hydration structure, overall structure of these compounds is understood by different molecular interactions in their aqueous solutions. The effect of temperature, presence of co-solutes, concentration of co-solutes on the partial molar volumes and compressibility of nucleic acid bases and nucleosides has been carried out. The review of literature and present development in the research area selected for the present work is given below. The review of literature covers thermodynamic properties and molecular interactions and developments in the present research area of nucleic acid bases and their nucleotides and ii) thermodynamic properties of different biologically active compounds in connection with the molecular interaction studies through volumetric, acoustical and transfer properties in general.

The partial molar isentropic and isothermal compressibilities of the nucleosides adenosine, cytidine, and uridine in aqueous solution at 298.15 K have been carried out by G. R. Hedwing, H. Høiland [1]. P. Rajput et al have studied temperature dependent physicochemical properties uracil, thymine and adenine in aqueous inositol solutions [2]. N. Kishor et al has been investigated the thermodynamic properties of nucleic acid bases and nucleosides in water and in aqueous glucose/sucrose solutions at 298.15 K [3]. R. N. Goldberg and et al have studied thermodynamics of the hydrolysis reactions of adenosine phosphate and phosphoenol-pyruvate at different temperatures [5]. G. R. Hedwig, et al have been carried out partial molar isentropic and isothermal compressions of the adenosine, cytidine,and uridine in aqueous solution at 298.15 K [6]. P. Hemmes, et al have studied solute-solvent and solute-solute interactions in aqueous solutions of bases, nucleosides, and nucleotides [9] Volumetric studies of nucleosides in aqueous solution are investigated by G. R. Hedwig [10]. T.S. Banipal et al investigated volumetric properties of nucleic acid bases and nucleosides in aqueous guanidine solutions at different temperatures [11]. P. Dyke, G. R. Hedwig studied the partial molar volumes and the partial molar heat capacities of cytidine, uridine, and adenosine in aqueous solution Brendon [12].

Furthermore, temperature dependent physicochemical properties of uracil, thymine and adenine in aqueous inositol solutions have been investigated by P. Rajput, Richu, T. Sharma, A . Kumar [14] and Tarlok S. Banipal, et al studied on nucleic acid bases and nucleosides in aqueous guanidine hydrochloride solutions for their thermodynamic properties [17]. The protein–nucleic acid interactions have been evaluated by R. Giambruno [18] and P. Sahaya

Amutha et al investigated partial molar volumes of aqueous biologically active compounds in aqueous solutions [21].

The volumetric properties such as partial molar and standard transfer volumes, acoustical properties like partial molar and transfer compressibilities, and other acoustical properties of different biologically active compounds have been studied by many researchers [4, 23, 26, and 27]. The viscosities and viscosity B-coefficients of bio-molecules have been carried out [4, 6, 8, and 19].

7. Rationale and Significance of the study

The reason and logic behind the selection of present research work and area for NABs and NABSDs is due to the significance of intermolecular interactions in solution as it is central importance to most chemical and biochemical disciplines. The exceptional importance of molecular recognition processes, both in chemistry and biology, makes the study of intermolecular interactions at the molecular level of fundamental significance for the understanding and rationalization of a great number of (bio)catalytic mechanisms. Intermolecular interactions may affect directly the reactivity of a (bio)molecule and can often be related to the observed selectivity of numerous (bio)catalytic processes.

The thermodynamic properties and viscometric studies of NABs and NABSDs in different aqueous solutions of cosolutes will disclose the different molecular level interactions among the components of solution including the dipole-dipole, ion-dipole, hydrogen bonding and hydration of solutes in the presence and absence of biologically active co-solutes. The volumetric studies related with the hydration volumes of solutes, compressibility of hydration structure of solutes and flow behavior studied by viscosity measurements as a result of different interactions reflects overall structure and orientation of solution in general and specific interactions in particular.

The study finds applications in the thermodynamic data, solubility of solutes, absorption of solutes in biological systems, in understanding solvent structure making/breaking ability of solutes and co-solutes and in chemical and pharmacological sciences.

8. Statement of aims and objectives of the work

In view of biological importance of nucleic acid bases (NABs) and their nucleosides (NABSDs), the present work is undertaken to study the molecular level interactions among NABs with water and different aqueous solutions containing relevant co-solutes by using measured densities, ultrasonic velocities and viscosities of the binary and ternary solutions at

different temperatures. In addition to this derived volumetric, acoustical and viscometric transfer properties of solutions will be studied and interpreted in terms of solute-solute, solute-solvent and solute-co-solute interactions.

Above investigation has following objectives with the mentioned hypothesis.

Objectives:

- To understand the molecular interactions between selected NABs and their sugar derivatives (NABSDs) with water and co-solutes in binary and ternary solutions
- To disclose the hydration structure of NABs and NABSDs in presence and absence of co-solutes
- To study the hydration structure and hydration behavior of NABs and NABSDs in different aqueous solutions of cosolutes
- To study the effect of temperature and concentration of co-solutes on volumetric, acoustical and viscometric properties of NABs
- To evaluate the structure making/breaking behavior of selected NABs and NABSDs in different aqueous solutions by viscosity B-coefficients

9. Hypothesis, Methodologies and Techniques to be adopted for the completion of the proposed work

Hypothesis:

- Molecular interactions among NABs and NABSDs with water and different aqueous solutions
- Change in the hydration structure of NABs and NABSDs in presence of cosolutes
- Variation in the thermodynamic properties like apparent and partial molar volumes and compressibilities of NABs and NABSDs in presence of cosolutes
- Effect of temperature and concentration of co-solutes on volumetric, acoustical and viscometric properties of NABs

Following Methodologies and Techniques will be adopted for of the proposed work:

- Volumetric methods – Densimetry by pycnometric method
- Acoustical methods – Ultrasonic velocity measurements using digital interferometer
- Optical methods – Refractive indices measurements using digital refractometer
- Viscometric methods – Viscosity measurements using Mansingh Surviscemeter
- Statistical methods – Statistical analysis of obtained data using MS-excel

10. Facilities required and availability at the Research Centre related to work proposed

Sr. No.	Name of the equipments/instruments	Availability
1.	Ultrasonic Interferometer (Mittal Enterprises, Model F-05, operating frequency 2 MHz)	Yes
2.	Anton Paar Abbemat 3200 compact, 131 digital refractometer	Yes
3.	Mansingh Survismeter	Yes
4	Electronic Balance	Yes
5.	Pycnometer	Yes
6.	Distillation Plant	Yes
7.	Thermostat	Yes

Relevant chemicals and glassware's are require for carrying out the present research. Some chemical are available with the school and remaining will be purchased from school budget for research.

11. Year wise Plan of the proposed work

Proposed work/Duration	First year	Second year	Third year
Course work and review of literature related to the proposed work, standardization of instruments			
Experimental work for NABs in different aqueous media and calculations, writing and communication of results to journals			
Experimental work for NABSDs in different aqueous media and calculations, writing and communication of results to journals			

12. Expected Research Outcome

The thermodynamic studies of NABs and NABSDs in different aqueous media are of great significance in chemical and biological field. This work will not only gives insights into the hydration structure, molecular interactions and structural properties of NABS and NABSDs in aqueous solutions but also disclose the different specific interactions and structure making/breaking nature of the solutes in solution. The work will produce the quality outcome in terms of rich data of thermodynamic properties of solutes like volumetric, acoustical and viscometric properties which will be effective for understanding the use of present solute for biological systems, understanding the absorption of solutes in biological systems and publication of research articles in reputed international journals. The results derived from the present work will be beneficial for the future researchers in this field.

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Research Scholar
(Mr. Rohidas V. Dudhate)
School of Chemical Sciences

Research Supervisor / Guide
(Dr. Santosh D. Deosarkar)
Professor
School of Chemical Sciences